MST e-NEWS

December 2015
Approved for public release;
distribution is unlimited.

INSIDE

Los Alamos
NATIONAL LABORATORY
EST. 1943

In a still image from the video, MST Division Leader David Teter introduces viewers to the Laboratory and its materials research.

Inset, the video being shown at the MRS Fall Meeting in Boston. In the image, Amy Clark and Seth Imhoff prep an experiment in the Materials Science Laboratory.

Shining a spotlight on Los Alamos's materials science

Movie on Lab's materials research shown at MRS Fall Meeting and Exhibit

The 2015 Materials Research Society Fall Meeting and Exhibit in Boston featured a new venue for the accomplishments of Los Alamos's materials scientists.

In addition to invited talks and poster presentations, the annual meeting and symposium included a five-minute movie, filmed at Los Alamos, showcasing Materials Science and Technology and Materials Physics and Applications division scientists discussing their work. MST Division Leader David Teter narrated the video, highlighting the Lab's mission of national security science and the opportunities available to early-career researchers.

> *"The insights we gain through the fundamental understanding of materials as well as discovering new materials is going to have a major impact on how we can change the world."*
>
> **David Teter**

The movie was shown in high-visibility locations including throughout the conference convention center, on conference hotel television channels, the MRS conference website, and YouTube. The MRS fall meeting draws on average 6,000 attendees, more than half of which are from the United States.

John Carpenter and Amy Clarke (Metallurgy, MST-6) brought viewers into the lab, introducing them to Los Alamos's additive manufacturing initiatives and the dynamic phase transformations studies enabling the materials of the future manufactured with this layer-by-layer printing technique.

continued on page 3

> I find this to be an exciting time where we are partnering with programs to define what future success looks like for the Laboratory in terms of people, equipment, facilities, and program.

From David's desk . . .

As we look forward to a strong and successful future for Los Alamos, the Laboratory is taking a much more active role in planning for that future, for example: the Purpose Statement, Los Alamos National Laboratory Goals, the five-year allocation zero exercise, and refreshing our Materials Strategy. I find this to be an exciting time where we are partnering with programs to define what future success looks like for the Laboratory in terms of people, equipment, facilities, and program. As many of you are aware, we initiated a refresh of the Materials Strategy through a number of Town Halls and feedback sessions to chart a course for our materials science R&D vision for the next 5-10 years. Soon we will be holding another Town Hall to articulate the potential changes in the Materials Strategy and scheduling Deep Dives to flesh out the details of the revised strategy. I highly encourage you to become engaged in these activities so that you can help us define the future of Los Alamos Materials.

MST-DO is leading a number of activities designed to grow our overall materials R&D portfolio consistent with MST and the Laboratory's mission. We have launched a Weapons Materials Strategy (led by Joe Martz) to identify R&D needs for the weapons program. The primary goal of this is to develop a new programmatic effort in NNSA to fund R&D in support of options for future life extension programs. A secondary goal has been to educate our next generation of materials scientists in weapons issues. Deniece Korzekwa has been leading an effort to develop a new program in Science Campaigns called Production Science aimed at ensuring we have the right kind of manufacturing tools and flexibility to make well-controlled samples for science experiments and sub-crits, but also to fund the science and R&D that is needed to support production issues and efficiencies. Lastly, I have continued to grow and develop materials programs in the Office of Energy Efficiency and Renewable Energy and the Office of Fossil Energy (FE), which has led to the Laboratory's involvement in the Lightweight Materials Consortium (led by Ellen Cerreta) and an anticipated program in Materials under Harsh Environments out of the Advanced Manufacturing Office and FE.

As we enter the holiday season, I would like to thank everyone in MST for their continued generous support of our local community through volunteer time and donations to this year's Employee Giving Campaign (~30% participation rate)! We also had a very successful Holiday Food and Gift Drive. It's great to see MST being so supportive of our local communities. The holidays can also be a stressful time of year with all of the various functions, gatherings, and preparations. Please take an extra moment at work to watch out for each other so that we can perform our work safely and securely. Although a co-worker may be distracted by this stress, we can help and protect each other.

I'd like to wish all of you and your families an enjoyable, relaxing, and happy holidays!

MST Division Leader Dave Teter

MRS cont.

Jennifer Hollingsworth, Nathan Mara, and Millie Firestone (Center for Integrated Nanotechnologies, MPA-CINT) explained the impact of their nanomaterials research to solve complex energy, medical, and information processing challenges.

Clarissa Yablinsky (Nuclear Materials Science, MST-16) being filmed in the Electron Microscopy Laboratory.

Carpenter and Mara gave invited talks at the meeting. Carpenter presented recent research on "Process Design for Control of Strength and Thermal Stability in Bulk Nanolamellar Copper-Niobium Composites Fabricated via Accumulative Roll Bonding," and Mara on "Interface Facilitated Deformation in Bimetallic Nanolayered Composites."

Other invited speakers from MST and MPA were Yue Liu (Materials Science in Radiation and Dynamics Extremes, MST-8) discussing "Strengthening Mechanisms of Highly Textured Cu/Co and Ag/Al Nanolayers with High Density Twins and Stacking Faults;" Romain Perriot (MST-8), "The Role of Chemistry and Disorder on Ionic Conductivity in Pyrochlore," Nan Li (MPA-CINT), "Measurement of Stress for Dislocation Motion through In Situ Nanoindentation;" Doan Nguyen (Condensed Matter and Magnet Science, MPA-CMMS) "Requirement of High Strength, High Conductivity Conductor and Reinforcement Materials for Ultra-High Field Pulsed Magnets;" Hou-Tong Chen (MPA-CINT) "Metasurfaces for Optical Antireflection and Polarization Manipulation;" Aiping Chen (MPA-CINT) "Role of Interfaces on Competing Interactions of Ferroic Films;" and Vivien Zapf (MPA-CMMS), "Complex Spin Textures in Functional Magnetic Materials." Enrique Martinez Saez (MST-8) co-chaired symposiums on microstructure evolution and mechanical properties in interface-dominated metallic materials and advanced atomistic algorithms in materials science.

See the video on YouTube: www.youtube.com/watch?v=h6SsjUBTVdw&index=31&list=PLGVe6BxyFHNX2RpSIgkJcuh502nXYLlrO.

John Carpenter discusses the Laboratory's additive manufacturing advances.

Long-term U-Nb experiments validate innovative thermodynamic and kinetic models for aging degradation and material processing

A decade-long experimental campaign to understand and predict thermal aging of uranium-niobium (U-Nb) alloys at Los Alamos recently provided unique data validating innovative thermodynamic and kinetics modeling. Uranium-niobium alloys behave similar to stainless steel, with good corrosion resistance and ductility in the time=0 condition, but suffer from severely degraded properties after thermal exposures. The phase transformations responsible for aging are quite complicated even though the alloy contains only two major elements. The significant body of experimental data gained at Los Alamos and elsewhere makes this material a good test case for critical comparisons of the theory of solid-state phase transformations with experiment. The insights gained will improve models of processing and aging of U-Nb and a wider variety of alloys.

Several hundred U-Nb alloy specimens were quartz-encapsulated and aged in the Sigma facility at Los Alamos under controlled conditions ranging from 100-625°C. Sampling the entire phase transformations pathway from time=0 to equilibrium required very long-term aging, up to five years. The microstructure was characterized by light and electron microscopy, while the phase amounts and compositions were measured by x-ray diffraction with full-pattern Rietveld analysis.

A companion multiscale modeling effort had two major aims: (1) update the thermodynamics and diffusion models for U-Nb, which undergirds simulations of engineering-relevant thermal treatments for both initial manufacture and in-service aging, and (2) gain fundamental scientific insight into the complex kinetics paths traversed by the system from time=0 to equilibrium.

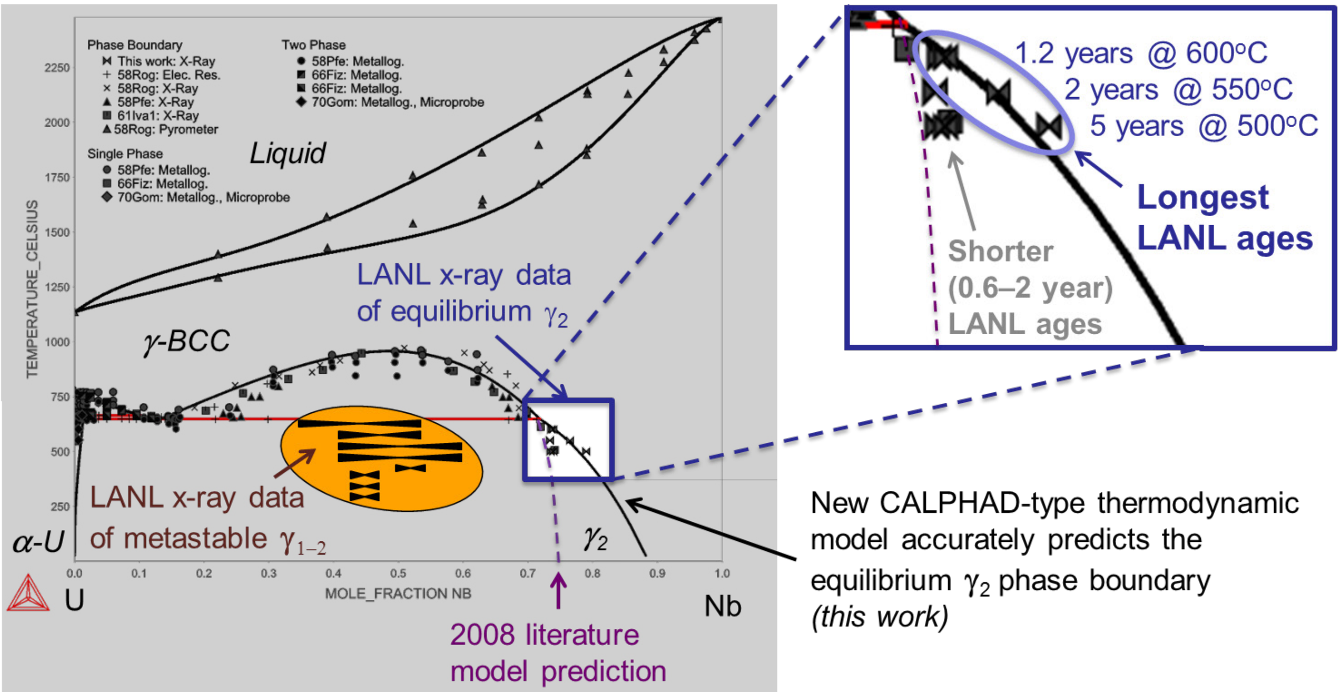
The first figure (next page) shows the updated equilibrium phase diagram. The new model was evaluated using the CALPHAD framework, which ensures an optimal fit accounting for both phase equilibria data (black data points) and thermochemical data (not shown). For the first time in this system, first-principles calculations (density functional theory) were incorporated into the overall assessment. The long-term Los Alamos aging data (inset) validated a key prediction of the model, the γ_2 phase boundary on the niobium-rich side, by bracketing the new model prediction.

Phase field simulations of microstructural evolution of the α (orthorhombic) and γ (body-centered cubic) phases—and more critically, their compositions—were run to better understand the complicated kinetic paths that lead to final equilibrium at temperatures between ambient and 647°C. As early as 1972, experiments revealed that the system

continued on next page

Long-term U-Nb experiments cont.

Updated U-Nb phase diagram



paused at a metastable phase, $\gamma_{1\text{-}2}$, of intermediate composition, ~50 atomic % Nb. This puzzling result has since been amplified by this study, shown in the orange region in the phase diagram figure. Since these compositions fall within the unstable region of the phase diagram (γ-BCC miscibility gap), a new approach was needed to explain observation of a persistent metastable $\gamma_{1\text{-}2}$ phase and the total phase transformations sequence. Phase field kinetics modeling was carried out, using as inputs the same thermodynamic model used to predict the phase diagram above, in addition to a variety of diffusion parameters also modeled in this study.

The next figure (page 5) shows phase-field kinetics simulations of a U-Nb diffusion couple at 450°C without (left) and with (right) the use of strain adjusted free energies in the simulation code. The vertical axis and color indicates the composition, and by extension the phase (blue has ~0 at.% Nb and is α-U, while turquoise, yellow, and red are richer in Nb and represent the γ-BCC phase.) As time increases (moving front to back), the alpha phase grows at the expense of the gamma phase, and the gamma increases its niobium content to conserve mass. How much the gamma composition changed was the major question. The results using the baseline thermodynamic model by itself (left side) failed to predict the $\gamma_{1\text{-}2}$ phase, and instead evolved the system straight to the equilibrium γ_2 phase. To explain the persistence of the $\gamma_{1\text{-}2}$ phase, the researchers hypothesized that strain energy between the misfitting α and γ crystal structures would shift Gibbs free energy of the γ-BCC phase in ways that would stabilize of the $\gamma_{1\text{-}2}$ phase. These modifications to the CALPHAD model (right) enabled improved phase-field predictions consistent with experimental evidence. The researchers conclude this is a plausible approach, one that might be applied to other actinide alloys and other engineering alloys more broadly.

The modeling portion of this work formed the PhD dissertation of Thien C. Duong, who successfully defended his thesis in October at Texas A&M University, with Robert Hackenberg (Metallurgy, MST-6) and Patrice Turchi (Lawrence Livermore National Laboratory, LLNL) serving as external examiners.

The experimental portion of the work was done at Los Alamos and funded through the NNSA Enhanced Surveillance Campaign (Tom Zocco, Los Alamos program manager). The work supports the Laboratory's Nuclear Deterrence and Energy Security mission areas, and the Materials for the Future science pillar by understanding and predicting the effects of material processing, aging, and corrosion on the properties, performance, and functionality of the materials, through a synergy of unique actinide R&D experiments coupled with multiscale modeling. The modeling portion of the work was funded through Lawrence Livermore, under the auspices of U.S. DOE under contract No. DE-AC52-07NA27344.

Reference: "A Hierarchical Computational Thermodynamic and Kinetic Approach to Discontinuous Precipitation in the U-Nb System, by Duong et al., "*Proceedings of the International Conference on Solid-Solid Phase Transformations in Inorganic Materials 2015.*

Los Alamos authors are Robert Hackenberg (MST-6), Heather Volz (Weapons Test Engineering, W-14), Anna Llobet

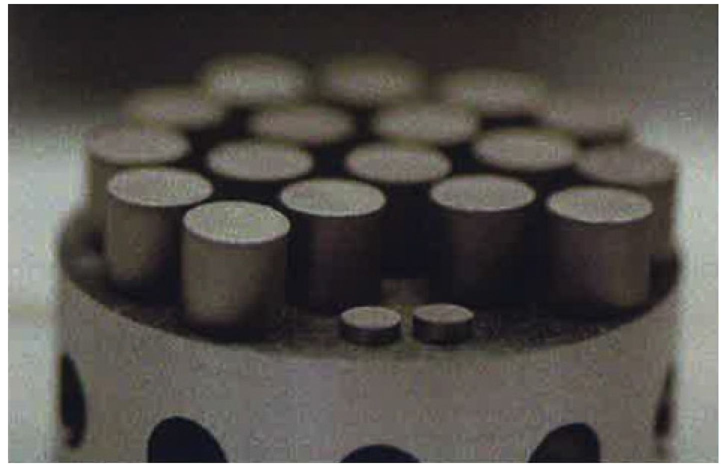
continued on next page

MST-7 plays national role in fabricating enriched uranium pellets for test irradiations of accident-tolerant nuclear fuels

Given Los Alamos's expertise in making high-density nuclear fuels and tailoring U-235 enrichments to match desired irradiation conditions, the Los Alamos Ceramic Nuclear Fuels Team (Engineered Materials, MST-7) was tasked with fabricating test articles for irradiation in Idaho National Laboratory's Advanced Test Reactor. It's part of a larger effort to create safer fuels for nuclear power plants.

The DOE Office of Nuclear Energy is partnering with the nuclear industry (Westinghouse, Areva, General Electric) to explore advanced accident-tolerant nuclear fuels that may offer both performance gains and a reduced risk of radioactivity releases in beyond design basis accidents. Many proposed concepts include nuclear fuel forms with limited or even no data about their performance under extreme environments (e.g., temperature, stress state, radiation levels). Verification of the irradiation behavior of these materials is critical to warrant further investment. The research includes less familiar fuel forms such as uranium mononitride (UN), and other fuels that have historically been limited to low-temperature, non-commercial reactors, such as uranium silicides and uranium borides.

Concepts under investigation by Westinghouse and Los Alamos include monolithic U_3Si_2 as well as fissile ceramic composite designs that propose to surround uranium mononitride with either U_3Si_2 or U_3Si_5. Composite designs deliver reactor performance improvements obtained by the higher uranium loading, while offering additional "coping time" before failure in the event of an off-normal condition.

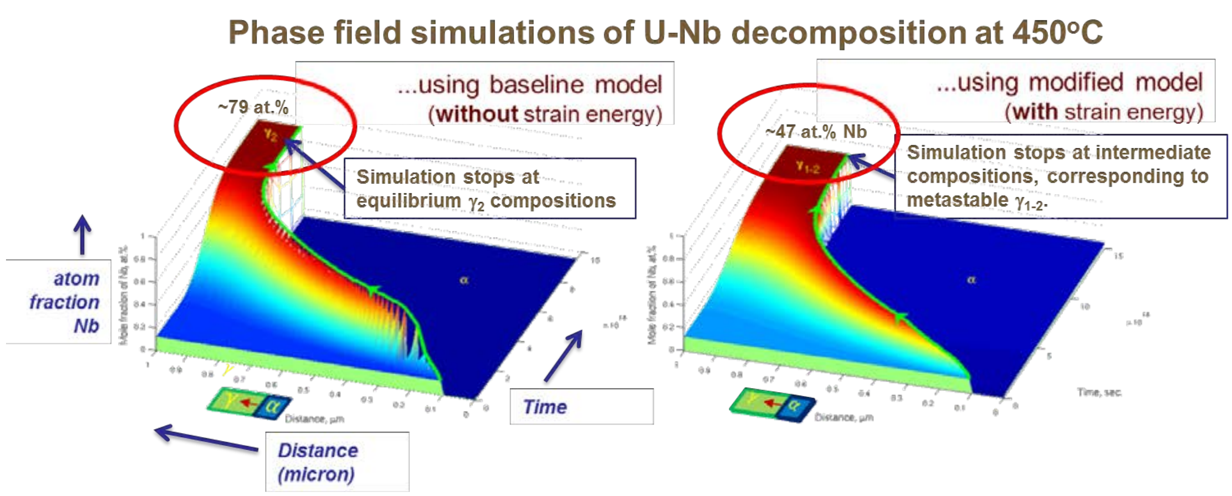


Enriched UN/U_3Si_2 pellets (8.4 mm right cylinders) and thermophysical property witness samples (foreground) fabricated in the MST-7 Fuels Research Laboratory for upcoming test irradiations at the Advanced Test Reactor. The UN/U_3Si_2 fissile ceramic composite concept is being investigated jointly by Westinghouse and Los Alamos, as supported by DOE-NE.

In FY15, the team produced kilograms of enriched material, which was fabricated into hundreds of pellets, at the Los Alamos Fuels Research Laboratory. The team fabricated enriched UN, as well as fissile ceramic composite UN/U_3Si_2 and UN/U_3Si_5 fuels. The fuel pellets included a range of U-235 enrichments and were sized to match commercial requirements and test irradiation conditions.

continued on next page

Long-term U-Nb experiments cont.



(Neutron Science and Technology, P-23), Alice Smith (Nuclear Materials Science, MST-16), and Graham King (Materials Science in Radiation and Dynamics Extremes, MST-8), with collaborators from Texas A&M University (Thien Duong, Raymundo Arroyave, Sean Gibbons), LLNL (Alex Landa and Patrice Turchi), California Institute of Technology (Saurabh Bajaj), and the Royal Institute of Technology in Sweden (Andrei Ruban and Levente Vitos). Tim Tucker, Pallas Papin, Bob Forsyth, Ann Kelly, Tim Beard, Jason Cooley, and Kester Clarke (all MST-6) contributed to the specimen preparation, aging, and characterization at Los Alamos.

Technical contact: Robert Hackenberg

MST-7 cont.

Josh White, John Dunwoody, Andy Nelson (MST-7), Darrin Byler, and Stewart Voit (Materials Science in Radiation and Dynamics Extremes, MST-8) executed the fabrication campaign, with support from Amber Telles, Michael Brand, and Erik Luther (Metallurgy, MST-6).

The DOE Office of Nuclear Energy funded the study via a cost share with Westinghouse. This work supports the Laboratory's Energy Security mission area and Materials for the Future science pillar.

In addition to the fabrication effort, the Los Alamos Ceramic Nuclear Fuels Team is also leading fundamental studies of these novel actinide materials. The team synthesized high-purity U_3Si, U_3Si_2, USi, and U_3Si_5, then characterized the thermophysical properties of these uranium silicide compounds. The data were added to models and simulations for upcoming test irradiations at Idaho and published by the *Journal of Nuclear Materials*. Although U_3Si and U_3Si_2 have seen historic use, previous assessments of thermal conductivity, heat capacity, and thermal expansion were limited to low temperatures and performed on materials that often contained significant impurity phases.

Development of powder metallurgy sintering routes, characterization of the resultant chemistry and microstructure, and thermophysical property measurement were performed by Josh White, John Dunwoody, and Andy Nelson. Synthesis of U-Si feedstock via arc melting was performed by Darrin Byler, James Valdez, and Ken McClellan (MST-8). Supplemental chemical and structural characterization were performed by Doug Safarik and Amber Telles (MST-6). This work was supported by the Office of Nuclear Energy's Advanced Fuels Campaign.

Technical contact: Andy Nelson

References:

A.T. Nelson et al. "Overview of properties and performance of uranium-silicide compounds for light water reactor applications." *Transactions of the American Nuclear Society* **110** (2014) 987-989.
J.T. White et al. "Thermophysical properties of U_3Si to 1150K," *Journal of Nuclear Materials* **452**, 304-310 (2014).
J.T. White et al. "Thermophysical properties of U_3Si_5 to 1773K," *Journal of Nuclear Materials* **456**, 442-448 (2015).
J.T. White et al. "Thermophysical properties of U_3Si_2 to 1773K," *Journal of Nuclear Materials* **464**, 275-280 (2015).
J.T. White et al. "Thermophysical properties of USi to 1673K," *Journal of Nuclear Materials*, under review.

Celebrating service

Congratulations to the following MST Division employees celebrating service anniversaries recently:

Lynne Goodwin, MST-7 .... 25 years
Rodney McCabe, MST-6 .... 15 years
Beverly Basey-Jones, MST-DO .... 10 years

Morrow featured in *JOM* young professional spotlight article

In a "Young Professional Technical Note," the August issue of *JOM* featured Ben Morrow (Materials Science in Radiation and Dynamics Extremes, MST-8) and his structural materials research. The article and a corresponding technical paper on in situ straining of magnesium were part of a larger feature on advanced characterization techniques using electron microscopy. *JOM* is a publication of The Minerals, Metals and Materials Society (TMS).

The mechanical behavior of hexagonal close-packed (hcp) metals is complex due to their relatively low crystal symmetry (compared with cubic materials), and dependence on both twinning and dislocation slip for ductility. Twinning, in particular, is an important aspect of plasticity in these materials, but the underlying mechanisms for twin nucleation, growth, and interaction with dislocations are still not completely understood. Researchers at Los Alamos have applied in situ mechanical testing using transmission electron microscopy (TEM) to characterize the motion of twin boundaries and study twin interactions with dislocations.

A Los Alamos-developed TEM in situ straining technique was used to probe the material and directly observe the mechanical behavior. It was previously known that the nucleation and growth of twins affected the dislocation structure, but the nature of the interaction and the mobility of the dislocations post-interaction were unknown. The researchers showed that new dislocations form inside the twins as they grow, challenging a common assumption that the dislocations are the result of the geometric conversion of dislocations outside the twins. Additionally, it was revealed that despite the drastic change in dislocation character as a result of interaction with a twin boundary, the dislocations themselves are still mobile. This information is critical to calibrating strength models that rely on appropriate representation of the activity and kinetics of plasticity mechanisms. This type of information is not accessible using traditional post-mortem techniques.

Funded by the Department of Energy, Office of Basic Energy Sciences, this work supports the Lab's Energy Security mission area and Materials for the Future mission pillar.

Technical contact: Ben Morrow

References:

"Young Professional Technical Notes: Ben Morrow Examines Advances in Structural Materials," *JOM* **67**, 8 (2015).
"Transmission Electron Microscope In Situ Straining Technique to Directly Observe Defects and Interfaces During Deformation in Magnesium," *JOM* **67**, 8 (2015), by Ben Morrow, Ellen Cerreta, and Carlos Tomé (MST-8), and Rodney McCabe (Metallurgy, MST-6).

Expanding career potential by learning from others' success

The Experimental Physical Sciences Directorate recently held a panel discussion on developing career opportunities for professional and administrative support staff.

Photo by Sandra Valdez, NIE-CS

Getting business done at the Laboratory relies critically on Los Alamos's professional and administrative support staff.

A panel discussion sponsored by the Experimental Physical Sciences Directorate (EPS) aimed to leverage the experiences of successful support staff to help others in building their career opportunities at the Lab.

"In EPS we want to create opportunities to enhance the professional development of our support staff. We hoped that hearing firsthand from others about their experiences would help grow awareness of different career paths possible at the Lab and important factors for career success," said Experimental Physical Sciences Associate Director Mary Hockaday. "These panelists shared important lessons—life lessons, really—about how to take control of those things you can control to keep your career on a positive track.

"The Lab is a system and its success depends on the contributions of everyone here," Hockaday said. "Enabling our staff members to reach their full potential is not only a good thing in itself, but also contributes to the success of the Laboratory and our national security mission."

The four panelists were Debbie Trujillo, a program manager for the National Security Office and Weapons Research Services; Charlene Martinez, a professional staff assistant for the Director's Office; Claudette Chavez, a technical project manager for Nuclear Materials Science; and Inez Valdez, of the Administrative Operations Team supporting Weapons Test Engineering. Their messages were conveyed in an overarching theme of positivity: look forward and not backward, treat others with respect, embrace and create opportunity, and always do your best.

HeadsUP!

Reminder: Call UPDATE hotline for latest on Lab operating status

When a snow storm or other wintry conditions are predicted, call the Lab's UPDATE hotline at 667-6622 or 1-877-723-4101 to hear the latest information on operating status before heading out to work. This information also will be put on the Lab's external/internal home page and provided to local television and radio stations, but your primary source for the Lab's current status is UPDATE.

Note: If you call the UPDATE hotline early in the morning and the message says the Lab is on "a regular operating schedule," call again just before leaving home, as the Lab's operating status may have changed in the interim. With above average snowfall predicted for Northern New Mexico this winter, employees are urged to stay abreast of changing weather conditions, prepare vehicles for winter-driving, and adjust driving speed for road conditions—remember, speed limits are meant for dry roads, not roads covered in snow and ice.

MSTe NEWS

Materials Science and Technology

Published by the Experimental Physical Sciences Directorate.

To submit news items or for more information, contact Karen Kippen, ADEPS Communications, at 505-606-1822, or kkippen@lanl.gov.

For past issues, see www.lanl.gov/org/padste/adeps/mst-e-news.php.

Los Alamos NATIONAL LABORATORY EST. 1943

LA-UR-15-29539
Approved for public release; distribution is unlimited.

Title:	MST e-News December 2015
Author(s):	Kippen, Karen Elizabeth
Intended for:	Newsletter Web
Issued:	2015-12-15